Vertical balance equations

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1 Block formulation

Let $\mathbf{x} \in \mathbb{R}^n$ be the "balanced variable" and $\mathbf{v} \in \mathbb{R}^n$ be the "unbalanced variable". They are linked through a "balance operator" $\mathbf{K} \in \mathbb{R}^{n \times n}$:

$$\mathbf{x} = \mathbf{K}\mathbf{v} \tag{1}$$

Let split $\mathbf{x}$ and $\mathbf{v}$ into m blocks, and $\mathbf{K}$ into m^2 square blocks:

$$\begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_m \end{pmatrix} = \begin{pmatrix} \mathbf{K}_{1,1} & \dots & \mathbf{K}_{1,m} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{m,1} & \dots & \mathbf{K}_{m,m} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_m \end{pmatrix} \tag{2}$$

or

$$\mathbf{x}_i = \sum_{j=1}^{m} \mathbf{K}_{i,j} \mathbf{v}_j \tag{3}$$

2 Triangular assumption

We assume that the balance operator $\mathbf{K}$ is block-lower-triangular, with identity diagonal blocks:

$$\mathbf{K} = \begin{pmatrix} \mathbf{I}_n & 0 & \dots & \dots & 0 \\ \mathbf{K}_{2,1} & \mathbf{I}_n & \ddots & & \vdots \\ \mathbf{K}_{3,1} & \mathbf{K}_{3,2} & \mathbf{I}_n & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \mathbf{K}_{m,1} & \mathbf{K}_{m,2} & \dots & \mathbf{K}_{m,m-1} & \mathbf{I}_n \end{pmatrix} \tag{4}$$

Thus, we can simplify equation (3) into:

$$\mathbf{x}_i = \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j + \mathbf{v}_i \tag{5}$$

3 Partial recursive inverse

Using the previous assumption, equation (5) can be transformed to compute $\mathbf{v}$ knowing $\mathbf{x}$ recursively:

$$\mathbf{v}_i = \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \tag{6}$$

It should be noted that the inverse of $\mathbf{K}_{i,j}$ is not required. This inverse formula is refered to as "partial" since the unbalanced variable $\mathbf{v}$ still appears on the right-hand side.

4 Full recursive inverse

We assume that for $1 \leq j \leq i-1$, $\mathbf{v}_j$ can be expressed as:

$$\mathbf{v}_j = \sum_{k=1}^{j} \mathbf{A}_{j,k} \mathbf{x}_k \tag{7}$$

where $\mathbf{A}_{j,k} \in \mathbb{R}^{n \times n}$. Plugging this expression into the partial recursive inverse formula (6), we get:

$$\begin{aligned}
\mathbf{v}_i &= \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \sum_{k=1}^{j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=1}^{j} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{k=1}^{i-1} \sum_{j=k}^{i-1} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \mathbf{x}_j \\
&= \sum_{j=1}^{i} \mathbf{A}_{i,j} \mathbf{x}_j
\end{aligned} \tag{8}$$

with:

$$\mathbf{A}_{i,i} = \mathbf{I}_n \tag{9}$$

$$\mathbf{A}_{i,j} = - \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \tag{10}$$

5 Statistical property

Since $\mathbf{v}$ is an "unbalanced variable", it has the following statistical property:

$$\text{if } i \neq j,\ \operatorname{Cov}\left(\mathbf{v}_i, \mathbf{v}_j\right) = 0 \tag{11}$$

6 Estimation with the partial recursive inverse

Using the partial recursive inverse (6) for $j < i$, we get:

$$\begin{aligned}
& \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_i\right) = 0 && (12)\\
\Leftrightarrow\ & \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{x}_i - \sum_{k=1}^{i-1} \mathbf{K}_{i,k} \mathbf{v}_k\right) = 0 && (13)\\
\Leftrightarrow\ & \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{x}_i\right) = \operatorname{Cov}\left(\mathbf{v}_j, \sum_{k=1}^{i-1} \mathbf{K}_{i,k} \mathbf{v}_k\right) && (14)\\
& \qquad = \sum_{k=1}^{i-1} \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_k\right) \mathbf{K}_{i,k}^{\mathrm{T}} && (15)
\end{aligned}$$

Using the statistical property (11) of $\mathbf{v}$, the term for which $k = j$ is the only one remaining in the right-hand side:

$$\begin{aligned}
& \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{x}_i\right) = \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right) \mathbf{K}_{i,j}^{\mathrm{T}} \\
\Leftrightarrow\ & \operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \mathbf{K}_{i,j} \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right) \\
\Leftrightarrow\ & \mathbf{K}_{i,j} = \operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1} && (16)
\end{aligned}$$

7 Expression with the full recursive inverse

Using the full recursive inverse (8) in the expression (16) of the balance operator', we get for $j < i$:

$$
\begin{aligned}
\mathbf{K}_{i,j} &= \mathrm{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) \mathrm{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1} \\
&= \mathrm{Cov}\left(\mathbf{x}_i, \sum_{k=1}^{j} \mathbf{A}_{j,k}\mathbf{x}_k\right) \mathrm{Cov}\left(\sum_{k=1}^{j} \mathbf{A}_{j,k}\mathbf{x}_k, \sum_{l=1}^{j} \mathbf{A}_{j,l}\mathbf{x}_l\right)^{-1} \\
&= \left(\sum_{k=1}^{j} \mathrm{Cov}\left(\mathbf{x}_i, \mathbf{x}_k\right) \mathbf{A}_{j,k}^{\mathrm{T}}\right) \left(\sum_{k=1}^{j}\sum_{l=1}^{j} \mathbf{A}_{j,k} \mathrm{Cov}\left(\mathbf{x}_k, \mathbf{x}_l\right) \mathbf{A}_{j,l}^{\mathrm{T}}\right)^{-1}
\end{aligned}
\tag{17}
$$

8 Practical computations

In practice, covariances are sampled from an ensemble. Let $\left\{\widetilde{\mathbf{x}}^1, \ldots, \widetilde{\mathbf{x}}^N\right\}$ be a set of N vectors that samples the distribution of $\mathbf{x}$ and $\left\{\delta\widetilde{\mathbf{x}}^1, \ldots, \delta\widetilde{\mathbf{x}}^N\right\}$ their centered counterparts:

$$\delta\widetilde{\mathbf{x}}^p = \widetilde{\mathbf{x}}^p - \langle\widetilde{\mathbf{x}}\rangle \tag{18}$$

where $\langle\cdot\rangle$ denotes the ensemble mean:

$$\langle\widetilde{\mathbf{x}}\rangle = \frac{1}{N}\sum_{p=1}^{N}\widetilde{\mathbf{x}}^p \tag{19}$$

The covariance $\mathrm{Cov}\left(\mathbf{x}_i, \mathbf{x}_j\right)$ can be estimated from these perturbations by:

$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N}\delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}} \tag{20}$$

The algorithm to compute the balance operator components using the partial recursive inverse equation (6) is detailed in algorithm 1. Its counterpart using the full recursive inverse equation (8) is detailed in algorithm 2. It should be noted that the first method requires storing the ensemble twice, while the second requires storing more matrices of size $n \times n$.

Algorithm 1 Recursive computation of the balance operator components using the partial recursive inverse formula

Copy the ensemble perturbations:
for $1 \leq p \leq N$ **do**
  $\delta\widetilde{\mathbf{v}}^p = \delta\widetilde{\mathbf{x}}^p$
end for

for $1 \leq i \leq m$ **do**
  for $1 \leq j < i$ **do**
    Estimate the cross-covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{v}}_j^p\right)^{\mathrm{T}}$$
    Inverse $\widetilde{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)$ to get $\widetilde{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$
    Estimate the balance operator component $\mathbf{K}_{i,j}$:
$$\widetilde{\mathbf{K}}_{i,j} = \widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right)\widetilde{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$$
  end for

  Update the unbalanced ensemble perturbation:
  for $1 \leq p \leq N$ **do**
    for $1 \leq j < i$ **do**
$$\delta\widetilde{\mathbf{v}}_i^p \leftarrow \delta\widetilde{\mathbf{v}}_i^p - \widetilde{\mathbf{K}}_{i,j}\delta\widetilde{\mathbf{v}}_j^p$$
    end for
  end for

  Estimate the auto-covariance of $\mathbf{v}_i$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_i\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{v}}_i^p \left(\delta\widetilde{\mathbf{v}}_i^p\right)^{\mathrm{T}}$$
end for

Algorithm 2 Recursive computation of the balance operator components using the full recursive inverse formula

Initialize the $\widetilde{\mathbf{A}}_{i,i}$ matrices:
for $1 \le i \le m$ **do**
  $\widetilde{\mathbf{A}}_{i,i} = \mathbf{I}_n$
end for

Estimate covariances of $\mathbf{x}$:
for $1 \le i \le m$ **do**
  for $1 \le j \le i$ **do**

$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}}$$

$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_j, \mathbf{x}_i\right) = \widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)^{\mathrm{T}}$$

  end for
end for

for $1 \le i \le m$ **do**
  for $1 \le j < i$ **do**
    Estimate the cross-covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:

$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \sum_{k=1}^{j} \widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_k\right) \widetilde{\mathbf{A}}_{j,k}^{\mathrm{T}}$$

    Inverse $\widetilde{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)$ to get $\widetilde{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$
    Estimate the balance operator component $\mathbf{K}_{i,j}$:

$$\widetilde{\mathbf{K}}_{i,j} = \widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) \widetilde{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$$

    Estimate the matrix $\mathbf{A}_{i,j}$:

$$\widetilde{\mathbf{A}}_{i,j} = -\sum_{k=j}^{i-1} \widetilde{\mathbf{K}}_{i,k} \widetilde{\mathbf{A}}_{k,j}$$

  end for

  Estimate the auto-covariance of $\mathbf{v}_i$:

$$\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_i\right) = \sum_{k=1}^{i}\sum_{l=1}^{i} \widetilde{\mathbf{A}}_{i,k} \widetilde{\mathrm{Cov}}\left(\mathbf{x}_k, \mathbf{x}_l\right) \widetilde{\mathbf{A}}_{i,l}^{\mathrm{T}}$$

end for